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MEMORANDUM FOR IN-HOUSE PUBLICATIONS

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SUBJECT: Authorization for Release of Technical Information, Control Number: AFRL-PR-ED-**TP-1998-095**
J. Harper, J. Sheehy, J. Mills and Bill Larson "Quantitative Analysis of the Condensation of B_JC_{n-J} Clusters (n = 2-12, J = 0,1,2) in Solid Argon" **HEDM Conference Presentation** **(Statement A)**

Quantitative Analysis of the Condensation of B_JC_{n-J} Clusters (n = 2-12, J = 0,1,2) in Solid Argon

J. Harper, J. A. Sheehy, J. D. Mills and C.W. Larson

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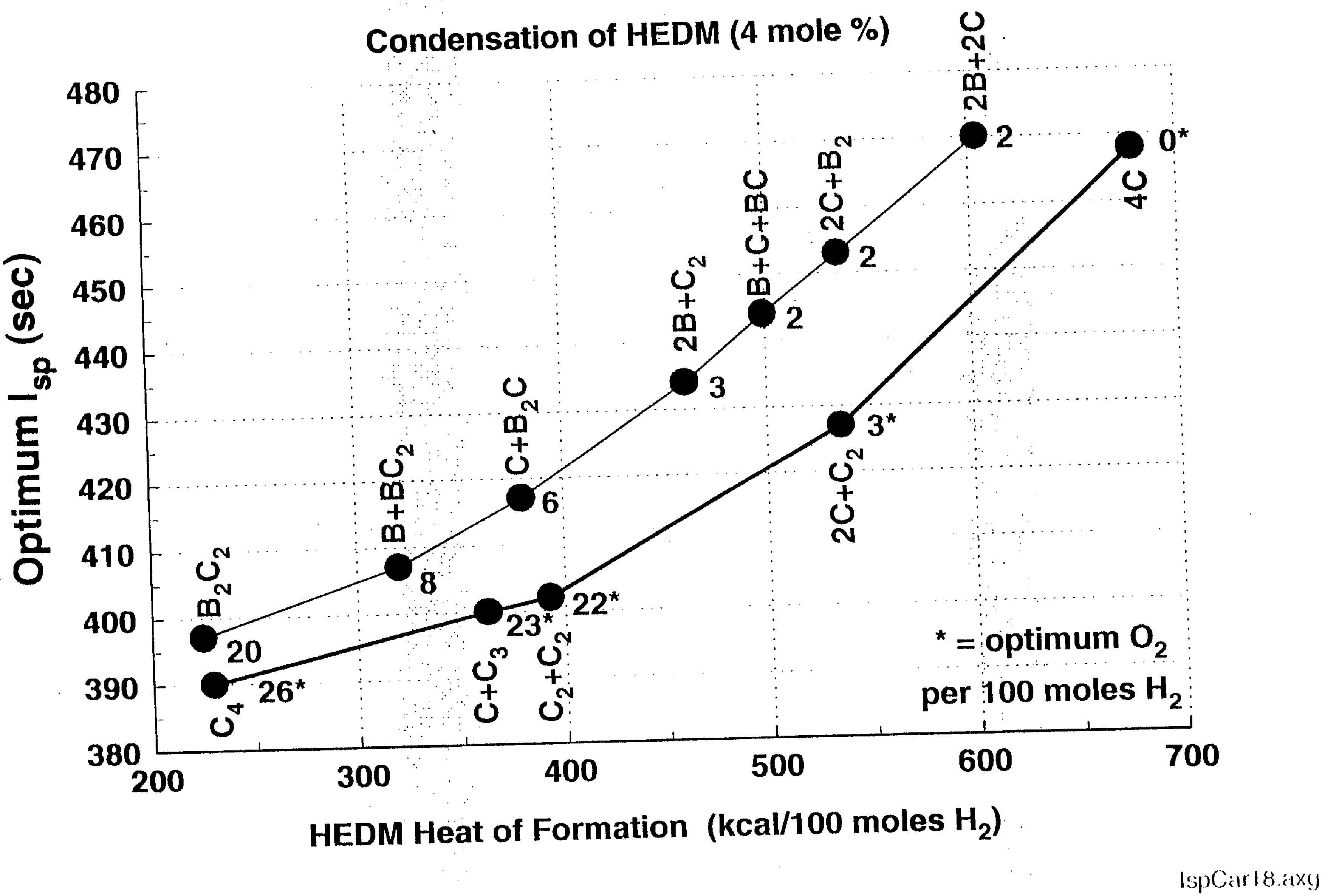
AFOSR HEDM Contractors' Conference
Monterey, California
20-22 May 1998



Condensation of HEDM (4 mole %)
Optimum I_{sp} (sec)
480
470
460
450
440
430
420
410
400
390
380
200
300
400
500
600
700
HEDM Heat of Formation (kcal/100 moles H_2)
B_2C_2
20
C_4
26*
$B+BC_2$
8
$C+B_2C$
6
$C+C_3$
23*
C_2+C_2
22*
$2B+C_2$
3
$B+C+BC$
2
$2C+B_2$
2
$2C+C_2$
3*
$2B+2C$
2
$4C$
0*
* = optimum O_2
per 100 moles H_2
IspCar18.axg

Objective - 5% atoms in cryogenic matrix

Approach

1. FTIR spectroscopy of B_JC_{n-J} clusters isolated in 10 K argon matrix

2. Ab-initio calculations of cluster
   (a) normal mode frequencies and frequency shifts of their isotopomers
   (b) infrared absorption intensities (km mol^{-1})

3. Measurement of cluster distributions produced upon deposition and after annealing . Absolute column densities (molecules cm^{-2}) from Beer's Law

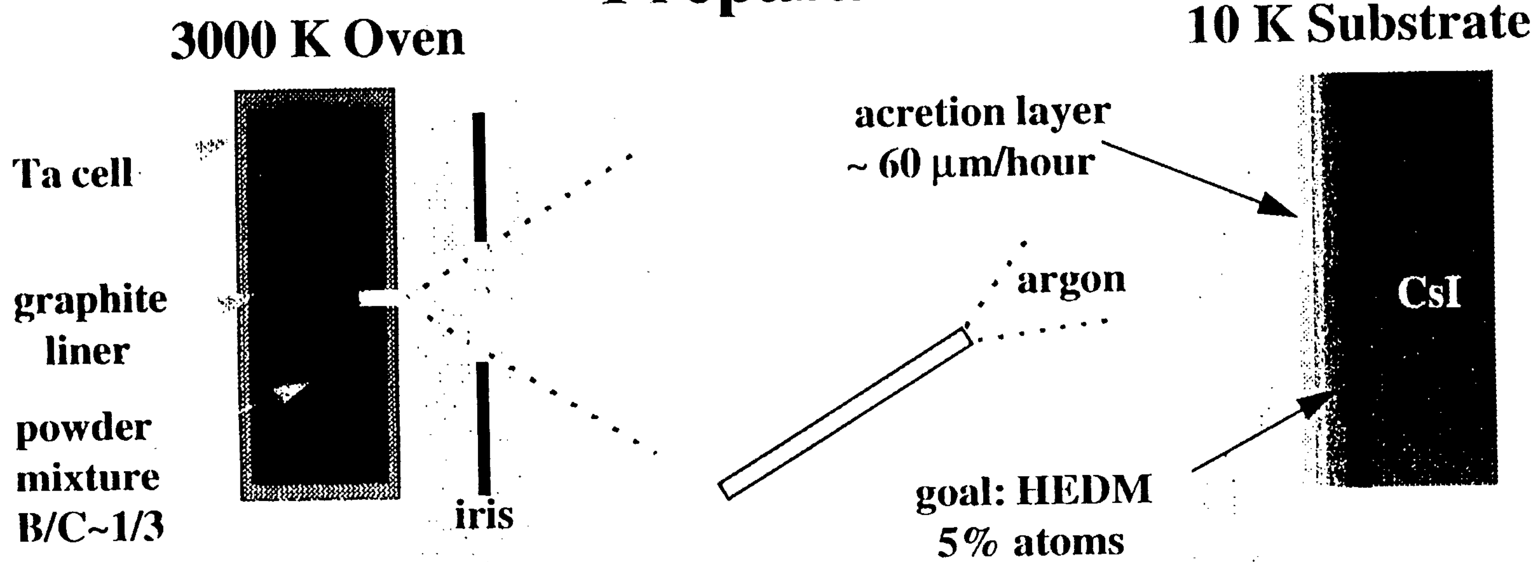
$$\langle \rho_i l \rangle = \frac{A_{exp}}{I_{theory}} N$$

$$A_{exp} = -\int_{\nu} \ln\left[\frac{E_t(\nu)}{E_0(\nu)}\right] d\nu$$

Summary of C_n and B_JC_{n-J} clusters identified or analyzed

		J			
cyclic-C_n	n	linear-C_n J = 0	J = 1	J = 2	J = 3
	2	C_2	BC	B_2	
	3	C_3	BC_2	B_2C	B_3
cC_4	4	C_4	BC_3	B_2C_2	B_3C
	5	C_5	BC_4	B_2C_3	B_3C_2
cC_6	6	C_6	BC_5	B_2C_4	B_3C_3
	7	C_7	BC_6	B_2C_5	B_3C_4
cC_8	8	C_8	BC_7	B_2C_6	B_3C_5
	9	C_9	BC_8	B_2C_7	B_3C_6
cC_{10}	10	C_{10}	BC_9	B_2C_8	B_3C_7
	11	C_{11}	BC_{10}	B_2C_9	B_3C_8
cC_{12}	12	C_{12}	BC_{11}	B_2C_{10}	B_3C_9
	13	C_{13}	BC_{12}	B_2C_{11}	B_3C_{10}

Preparation

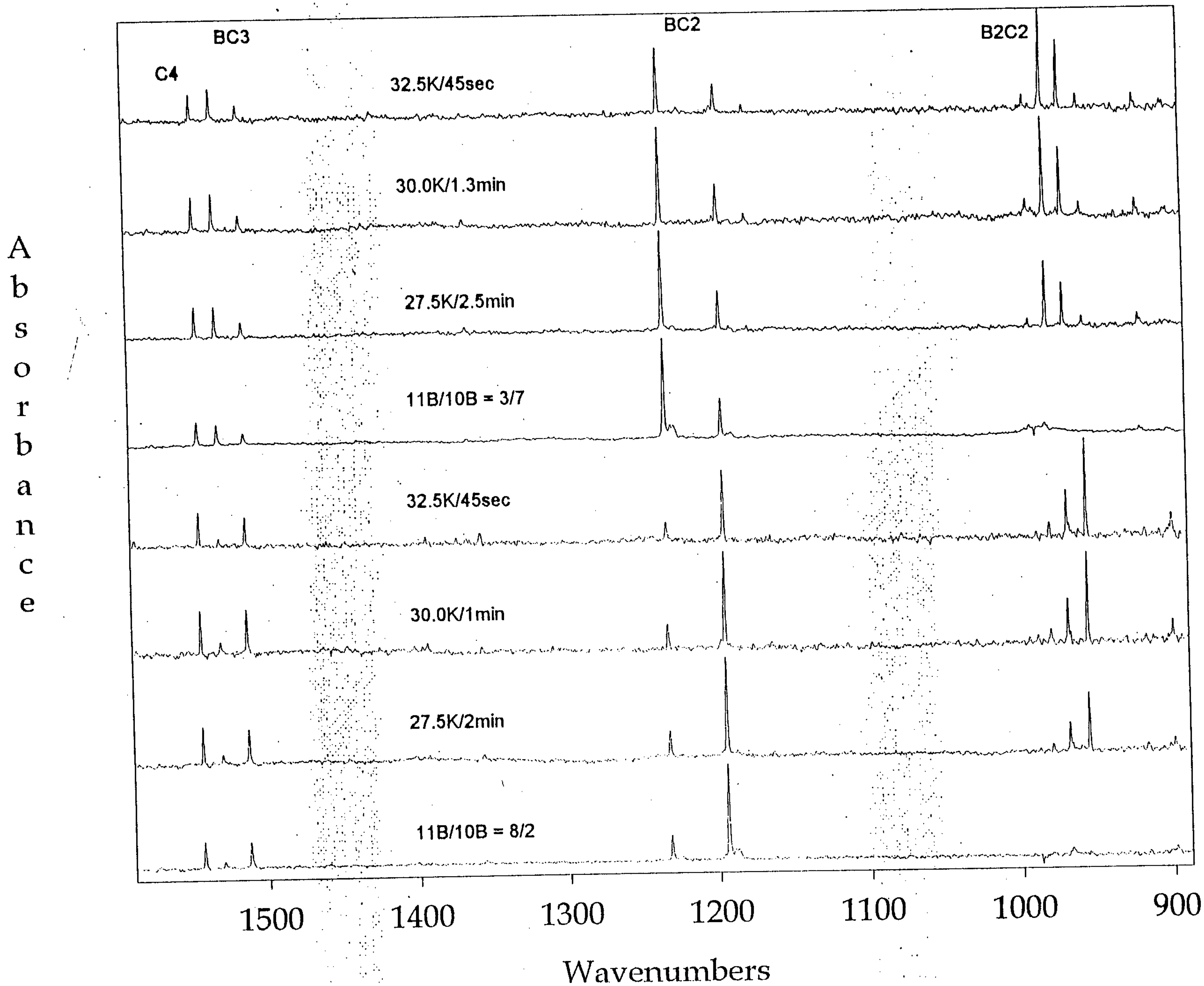


Annealing

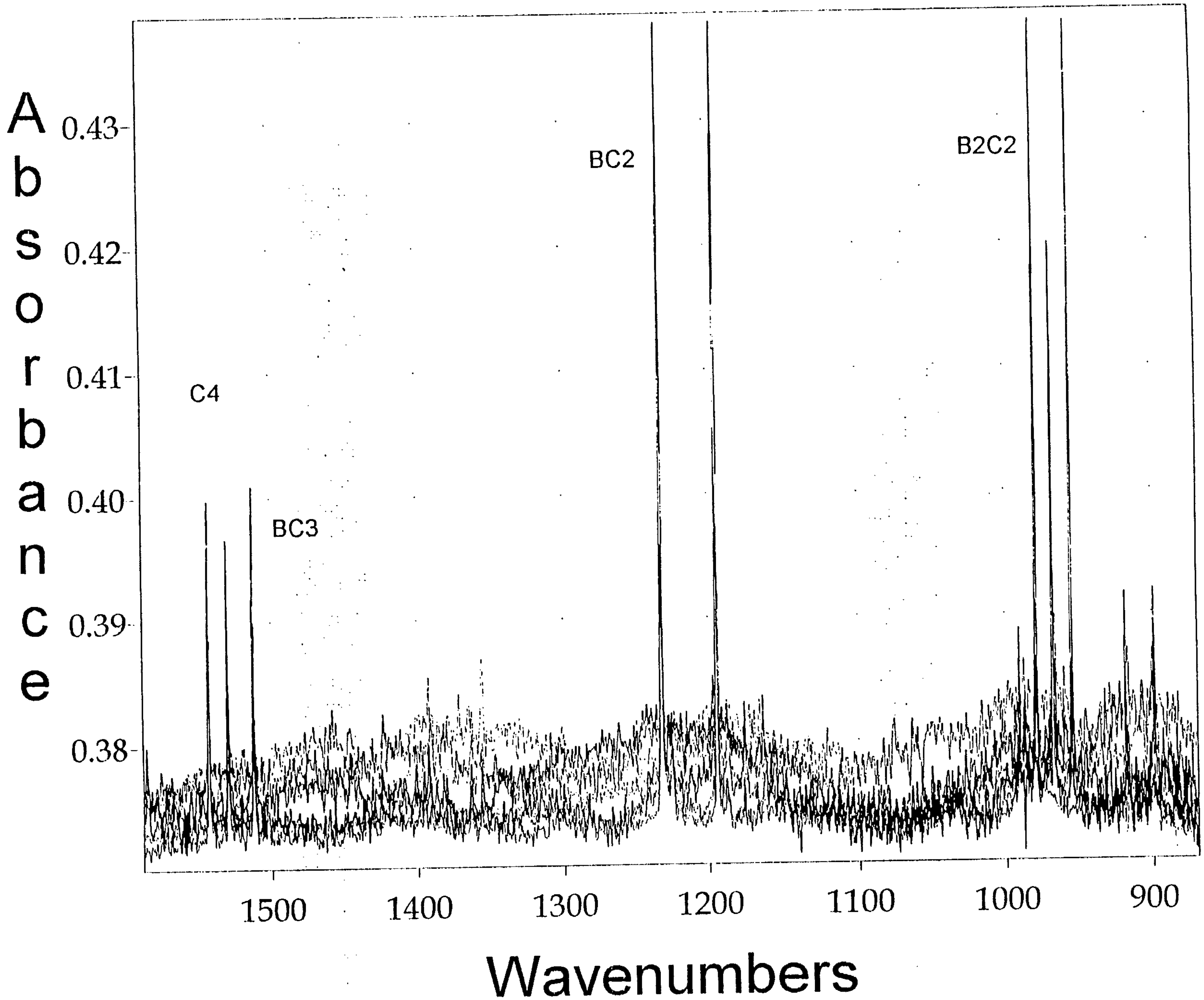
<u>a0</u> 10 K	<u>a3</u> 32.5 K, 60 s	<u>a6</u> 40.0 K, 20 s
<u>a1</u> 27.5 K, 120 s	<u>a4</u> 35.0 K, 45 s	sublimation
<u>a2</u> 30.0 K, 90 s	<u>a5</u> 37.5 K, 20 s	rate ~ 1 μm/s

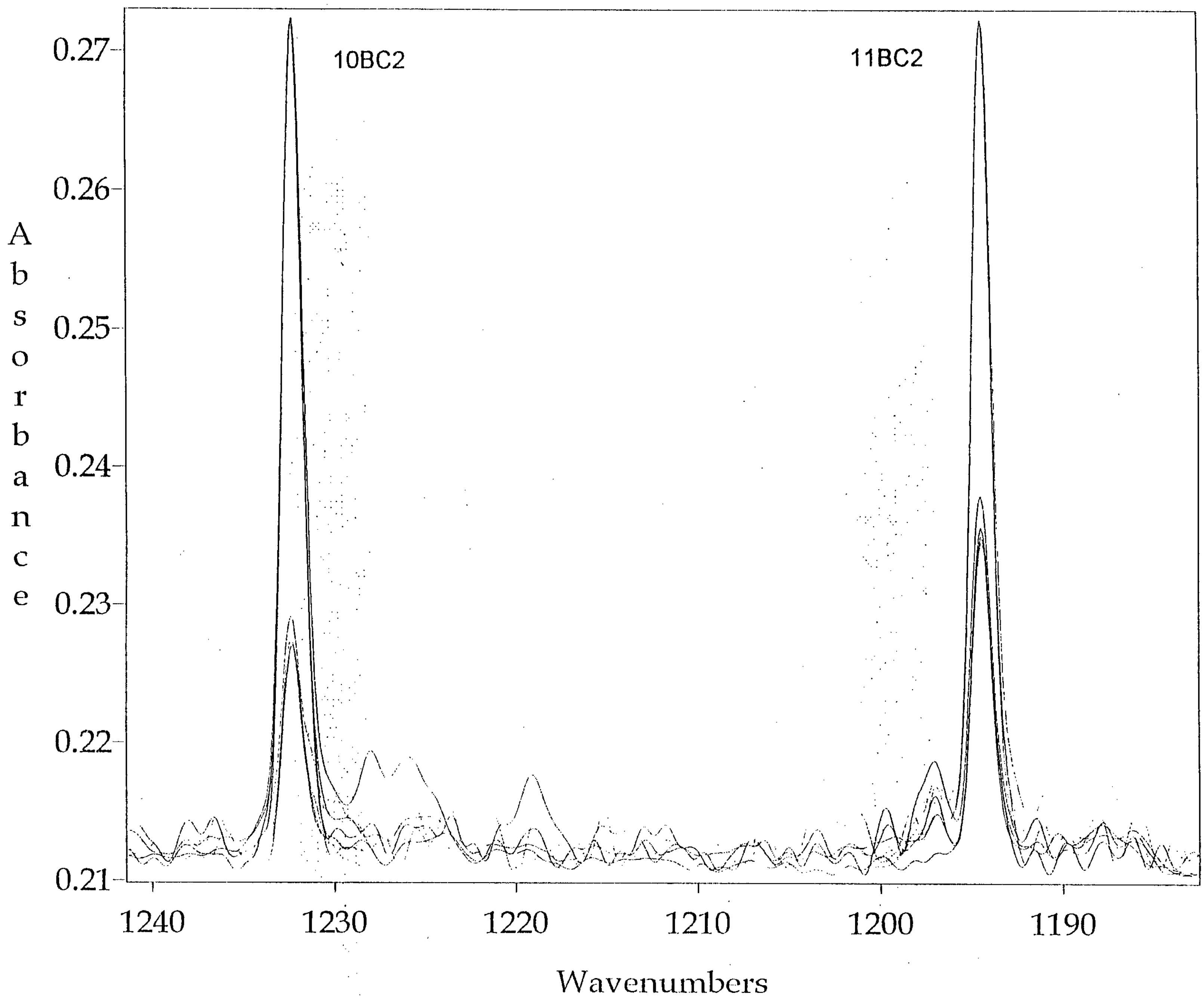
Precision matched pair of matrices

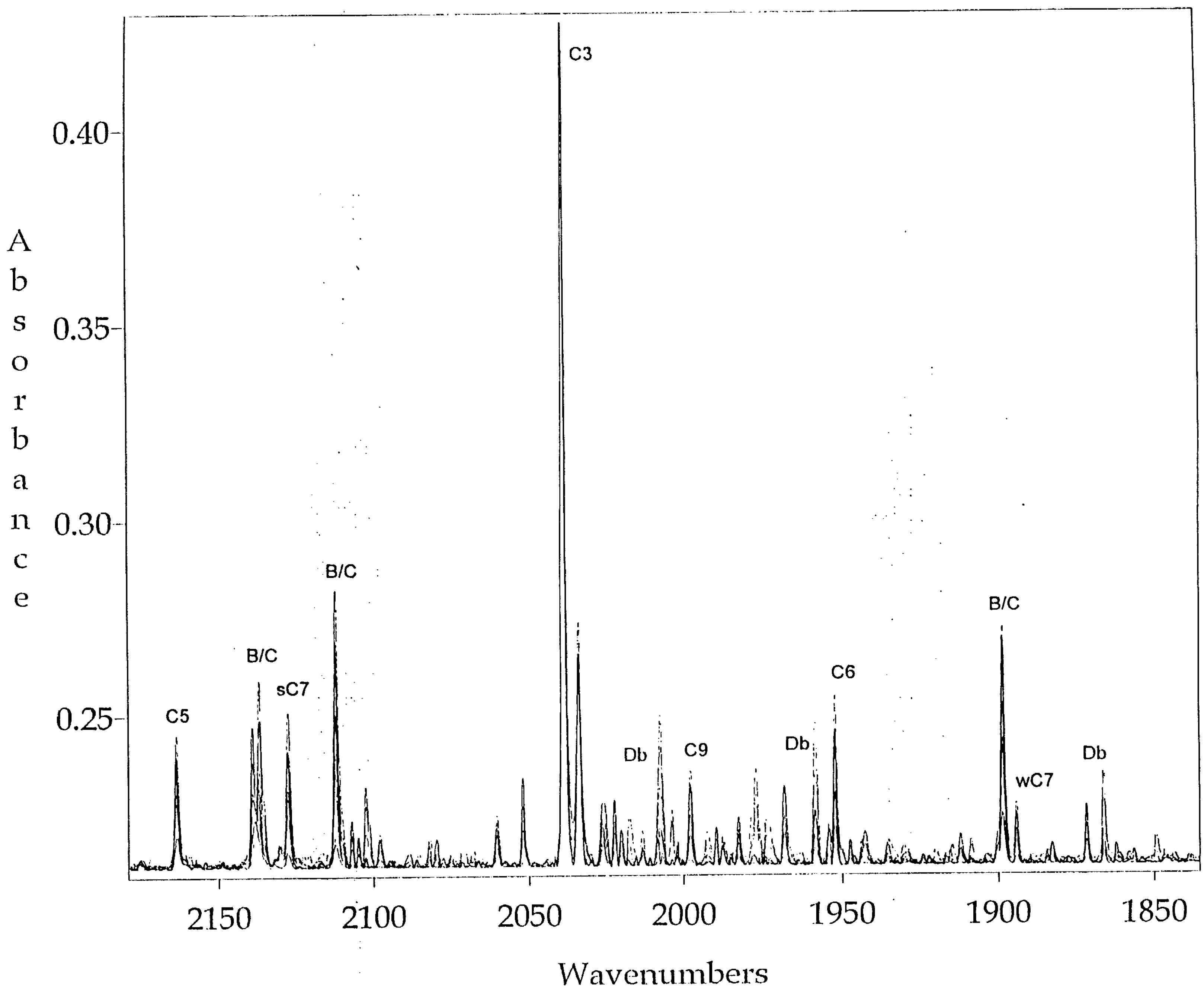
Green Matrix	$^{11}B/^{10}B = 80/20$	enhanced $^{11}B_JC_{n-J}$
Red Matrix	$^{11}B/^{10}B = 27/73$	enhanced $^{10}B_JC_{n-J}$

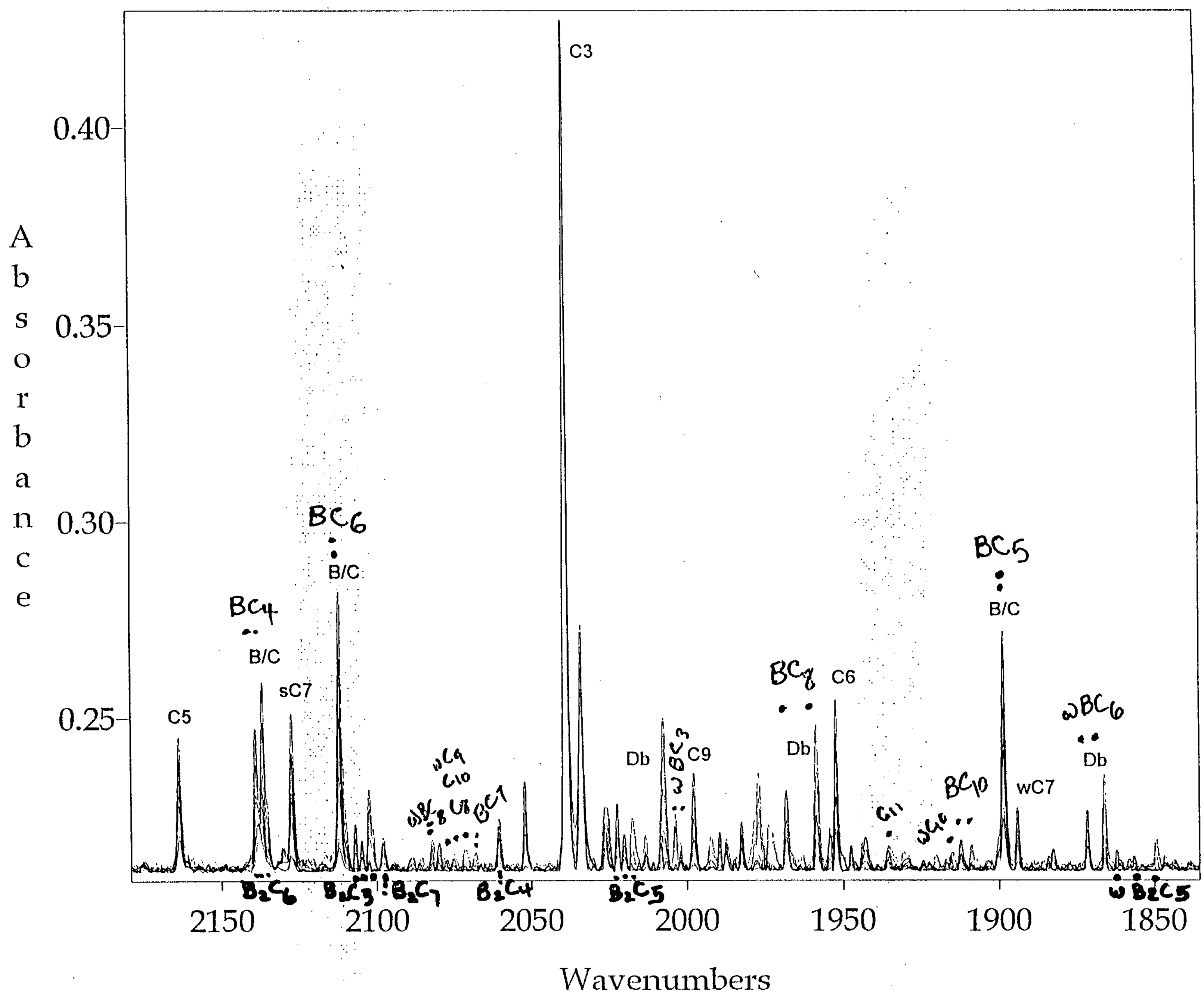


C4
BC3
BC2
B2C2
32.5K/45sec
30.0K/1.3min
27.5K/2.5min
11B/10B = 3/7
32.5K/45sec
30.0K/1min
27.5K/2min
11B/10B = 8/2
Absorbance
1500
1400
1300
1200
1100
1000
900
Wavenumbers

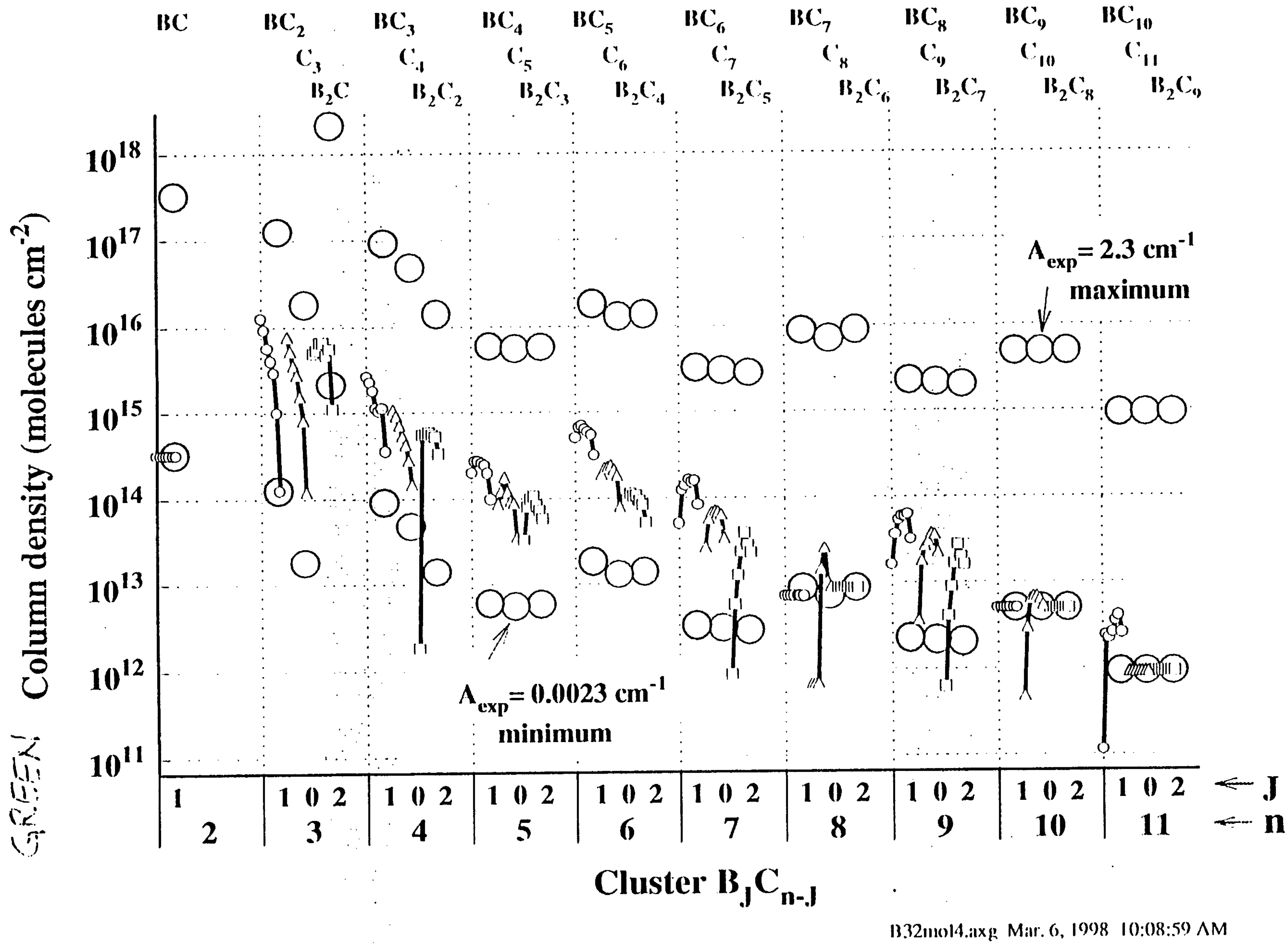

Absorbance
0.43
0.42
0.41
0.40
0.39
0.38
C4
BC3
BC2
B2C2
1500
1400
1300
1200
1100
1000
900
Wavenumbers


10BC2
11BC2
Absorbance
0.27
0.26
0.25
0.24
0.23
0.22
0.21
1240
1230
1220
1210
1200
1190
Wavenumbers

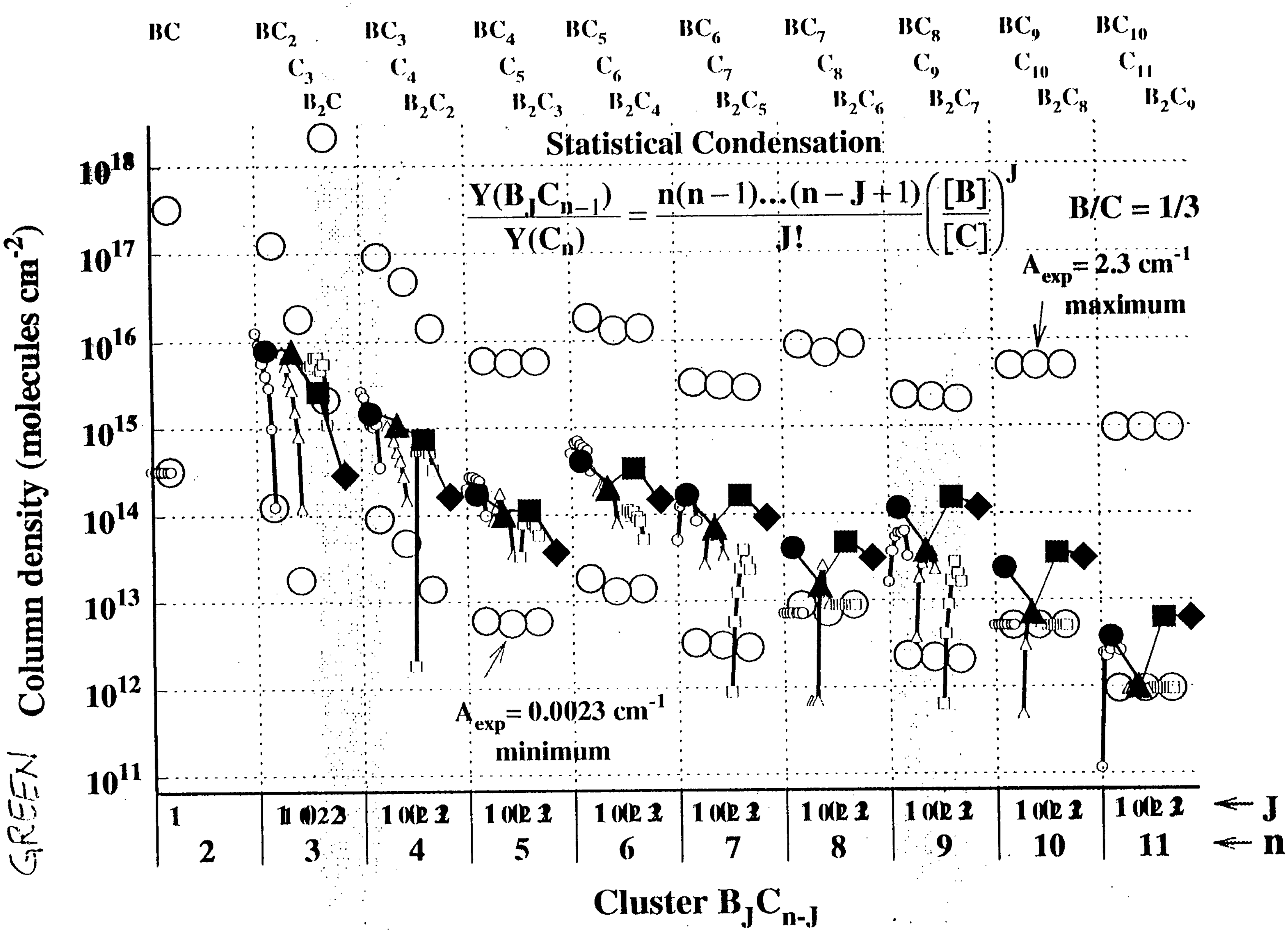

Absorbance
0.40
0.35
0.30
0.25
C3
B/C
B/C
sC7
C5
Db
C9
Db
C6
B/C
wC7
Db
2150
2100
2050
2000
1950
1900
1850
Wavenumbers



C3
C5
BC4
B/C
sC7
BC6
B/C
C6
C9
Db
Db
BC5
B/C
wC7
wBC6
Db
BC10
Wavenumbers
Absorbance



BC
BC_2
C_3
B_2C
BC_3
C_4
B_2C_2
BC_4
C_5
B_2C_3
BC_5
C_6
B_2C_4
BC_6
C_7
B_2C_5
BC_7
C_8
B_2C_6
BC_8
C_9
B_2C_7
BC_9
C_{10}
B_2C_8
BC_{10}
C_{11}
B_2C_9
Column density (molecules cm^{-2})
10^{18}
10^{17}
10^{16}
10^{15}
10^{14}
10^{13}
10^{12}
10^{11}
$A_{exp}= 2.3\ cm^{-1}$
maximum
$A_{exp}= 0.0023\ cm^{-1}$
minimum
1 1 0 2 1 0 2 1 0 2 1 0 2 1 0 2 1 0 2 1 0 2 1 0 2 1 0 2 ← J
2 3 4 5 6 7 8 9 10 11 ← n
Cluster B_JC_{n-J}
B32mol4.axg Mar. 6, 1998 10:08:59 AM
GREEN



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Conclusions

1. C_3 is linear but BC_2, B_2C and B_3 are cyclic.

2. $n > 3$; $J = 0, 1, 2$ clusters are linear. Boron atoms cap the ends of linear chains.

3. $J = 0, 1, 2$ substitution in $n \geq 5$ clusters does not significantly affect IR intensities.

4. For $n \geq 5$ the absorption intensity of even n clusters is two to three times smaller than that of odd n clusters.

5. B_2C_2 grew most dramatically upon annealing. BC was not detected. Its upper limit column density is comparable to that of $n = 4$ clusters. B_2C_2 sources may be $2BC$ or $B + BC_2$ but $C + B_2C$ does not form B_2C_2.

6. $n = 3, 4$; $J = 0, 1$ clusters disappear upon annealing but $J = 2$ clusters either grow or remain unchanged. Capping the ends of clusters with boron seems to render them inert to further condensation.

7. Statistical cluster distributions are apparent in $n = 4$ and 5 clusters. B_2C yields are too high and B_2C_{n-2} yields are too low in larger $n \geq 6$ clusters.

8. $n \geq 5$ clusters grow upon annealing and larger clusters grow more than smaller clusters.